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Inversion of the Spatially Varying Parameters in a Marine Ecosystem Model

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Abstract

The adjoint variational method is applied to numerical simulation of marine ecosystem dynamics on global scales based on the spatial parameterization in this study. On the basis of previous studies, we make improvements and conduct discussion in detail by assimilating chlorophyll-a data into a simple NPZD model. When the spatially varying V_m (Maximum uptake rate of nutrient by phytoplankton) is estimated alone, new strategies are designed to optimize the step-length that is used to adjust the parameters preferably and the assimilation efficiency is improved. On the condition that the same step is employed, the reduced cost function (RCF), the mean error of phytoplankton in the surface layer (ME), the absolute average error (AAE) and the relative average error (RAE) of V_m between given and simulated values decrease obviously compared with strategy in previous work. How the distribution schemes of spatial parameterization and influence radius affect the results is discussed by utilizing the above strategy, and the optimal influence radius corresponding to each distribution scheme is obtained. On the basis of the above work, when the five key parameters are estimated separately, the two given types of spatial variations could be reproduced and the RAE are less than 3%. It demonstrates that the simulation precision and computing efficiency could be improved by utilizing the improved strategy to modify the step-length and by using the optimized distribution schemes of independent grids.

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1. Introduction

Numerical simulation which allows us to synthesize our knowledge is invaluable to the marine ecosystem that is significant in the progress of marine science research and global climate change. Marine ecological numerical simulation within the scope of global has advanced rapidly with the development of more complex models as the field expands, which provides logical explanations of data and makes up for insufficient observations to provide a basis for prediction and forecasting [1]. To a large extent, parameter values in marine ecosystem models that are hard to define accurately can strongly affect model performance and the simulated results may change a lot due to microvariation of parameters. So optimizing parameters becomes more and more important in numerical simulation of marine ecosystem dynamics.

Researches of the last 20 years show that adjoint assimilation method that combines variational principles with optimal control theory is an effective tool to optimize parameters [2]. It chooses marine dynamic equations as constraint conditions, and constructs cost function defined as differences between simulated quantities and measured quantities. The gradients of the cost function with respect to the tunable input variables of the model is solved by using a set of so-called “adjoint equations” derived from the model equation with adjoint operator method or Lagrangian multiplier method. Then the gradient is used in an iterative gradient-descent algorithm to optimize the value of the input variables and maximize the agreement between model and observations which achieves the estimation of marine elements that cannot be observed. Lawson et al. [3] first illustrated that adjoint method represented a powerful approach for recovering model parameters as well as initial conditions by applying it to a simple predator-prey model. Gunson et al. [4] applied variational data assimilation to a coupled physical-biological model of the North Atlantic and recovered model parameters successfully by assimilating satellite ocean color data in different biological areas simultaneously. They indicated that it becomes possible to successfully constrain all ecosystem parameters at once. The variational adjoint technique was applied to a five-component ecosystem model of central equatorial Pacific by Friedrichs [5], which effectively minimized the misfits between model and data by adjusting six model parameters. Tjiputra et al. [6] used a three-dimensional global ocean biogeochemical cycle model on the basis of five-year seasonal climatology of SeaWiFS Level 3 chlorophyll data and seasonal in situ surface nitrate data provided by WOA. They pointed out that the adjoint model was capable of optimizing sensitive parameters and carbon fluxes in the euphotic zone. Ward et al. [7] studied the efficacy of the variational adjoint method and microgenetic algorithm with respect to the calibration of two simple one-dimensional models for Arabian Sea data.

On the other hand, it is questionable to take ecological parameters to be constant especially in the global scope because marine ecosystem responds to changes in environmental conditions and different species included in the model state variables are affected differently by environmental biotic and abiotic changes [6, 8-10, and 11]. There have already been several studies focusing on this problem. The results of Losa et al. [12] and Hemmings et al. [13] exhibited significant spatial variations in biological parameters, but the models and observations were not considered as a whole. Refer to Fan and Lv's [14] introduction for details. For the improvement purpose, Fan and Lv [14] assimilated SeaWiFS chlorophyll-a data into a simple NPZD model by the adjoint method in a climatological physical environment provided by FOAM. They selected five tunable parameters that are sensitive to the modeling status and uncorrelated with each other by sensitivity analysis, and then explored a new method to invert parameters in which several grids are selected as independent grids in the research area and the parameter values of other grids can be represented through linear interpolation of these independent grids. The

feasibility of utilizing spatial parameterizations and the validity of adjoint model were justified, but their work is just a beginning and needs further improvement.

In this paper, we applied the adjoint variational method to numerical simulation study of global marine ecosystem on the basis of the work of Fan and Lv [14] and spatially varying parameters are estimated by twin experiments. Background field, data, model and setting of the twin experiments are introduced in Section 2, and we design the strategies which are used to define the value of step-length to adjust the parameters preferably and improve assimilation efficiency in Section 3. How the distribution schemes and influence radius of spatial parameterization affect the results are discussed by using the optimal strategy in Section 4. Two given spatial variational types of the five key parameters are inverted separately, and they are described in Section 5. At last we give the conclusion.

2. Model and experiment design

2.1. Background filed

The ecosystem model is driven by a stable physical environment that is climatologically monthly mean data including circulation and water temperature provided by Fast Ocean-Atmosphere Model (FOAM) version 1.5, a fully coupled global ocean-atmosphere model [15].

2.2. Model and control variable selection

The ecosystem model in this study is a nitrogen-based NPZD model whose detail information is given in previous studies [16, 17]. Marine ecosystem models typically involve a large number of parameters and only a subset of those parameters is sensitive to the modeling status. On the other hand, high correlations may exist between many parameters because of the inherent nonlinearities. Friedrichs et al. [18] explained that two highly correlated parameters cannot be simultaneously estimated successfully. Therefore, the correlation between the parameters and parameter sensitivities must be studied. In previous study [14], five parameters are selected as control variables based on two methods (by a conventional sensitivity analysis and investigating the gradients of the cost function with respect to each parameter, respectively). In this paper, these parameters (Vm , Gm , Dz , Dp and e) still serve as control variables and their initial values are listed in Table 1.

Table 1. Key ecological parameters and their initial values in the model.

Symbol	Parameter	Initial value	Unit
Vm	Maximum uptake rate of nutrient by phytoplankton	1.0	day ⁻¹
Gm	Zooplankton maximum grazing rate	0.5	day ⁻¹
Dp	Phytoplankton mortality rate	0.1	day ⁻¹
Dz	Zooplankton mortality rate	0.05	day ⁻¹
e	Remineralization rate of detritus	0.0212	day ⁻¹

Based on the initial values CV^0 of the ecological parameters listed in Table 1, two given types of parameter variations are constructed as the follow formulas (see Fig. 1).

$$CV(lat) = (-lat^2/16200 + 1.25) \cdot CV^0 \quad (1)$$

$$CV(lat) = (lat^2/16200 + 0.75) \cdot CV^0 \quad (2)$$

CV is the parameter value scaled by the corresponding value listed in Table 1, and it is a function of latitude. According to the formations of the two given types, the parameters under estimation show a variation of parabola type symmetrical about the equator between 0.75 and 1.25 (scaled values), because the solar radiation is symmetrical between north and south on the earth and the temperature varies with different latitudes to a certain extent.

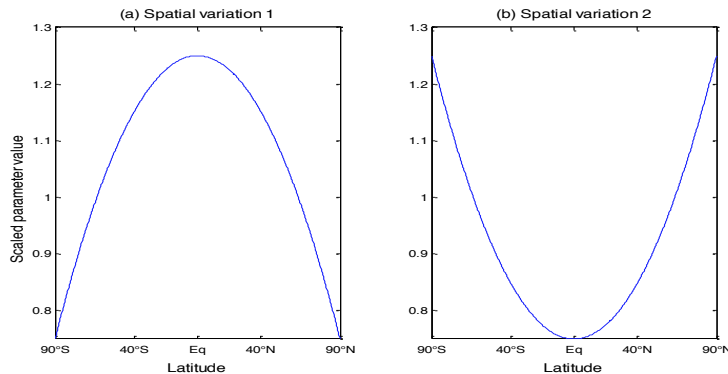


Fig. 1. The two given types of parameter variations.

2.3. Diffuse attenuation coefficient

Diffuse attenuation coefficient for the Photosynthetically Available Radiation in Case-1 waters, denoted by $K_d(PAR)$ is expressed as the form of Eq. (1); note that PAR is the polychromatic radiation within the entire 400–700 nm spectral range. $K_d(490)$ is the diffuse attenuation coefficient for Case-1 waters when the wavelengths of light is 490 nm and the adopted constant for pure water is 0.0166 m^{-1} , obtained by using $[Chl]$ as an intermediate tool [19]. The $K_d(PAR)$ values for the whole simulated area is shown in Fig. 2 calculated by using the SeaWiFS monthly mean data (averaged over 1998–2001) in January.

$$K_d(490) = 0.0166 + 0.0773 \cdot [chl]^{0.6715}$$

$$K_d(PAR) = 0.0864 + 0.844 \cdot K_d(490) - 0.00137/K_d(490) \quad (3)$$

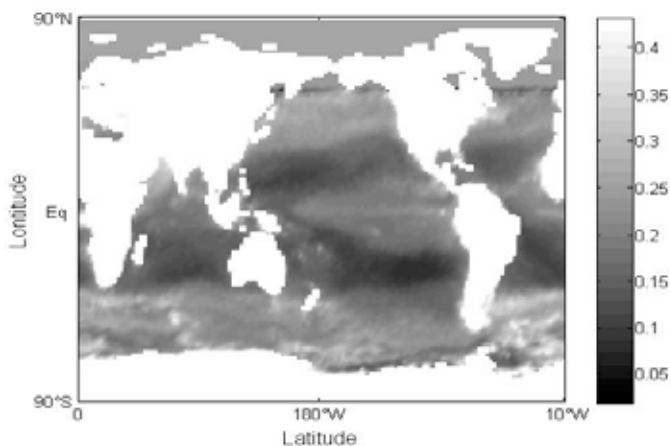


Fig. 2. $K_d(PAR)$ calculated by using Eq. (3) and [Chl] values obtained through the SeaWiFS monthly mean data in January.

2.4. Experiment design

Fan and Lv [14] run the model for 10 years to achieve a steady annual cycle and data in January in this status is used to provide the initialization. Run the model for five days and the modeled data of phytoplankton in the surface layer are memorized as model generated ‘observations’ for the twin experiments in this study because the influence to the simulation result is very small by using data in different month as initialization. Hereafter, these ‘observations’ are assimilated into the model to estimate the given spatial variations of the parameters. The integral time-step is 3 hours and the assimilation step is 28 in all experiments. The spatial parameterizations is done in such a way that several grids are selected as independent grids for which the parameter values are independent, and then the parameter values of other grids could be obtained by a linear combination (such as Cressman interpolation) [20]. The distributions of the independent grids are introduced in each experiment. We evaluate the experiment results by comprehensive analysis of RCF, the ME and the misfit of the estimated parameter including AAE and RAE.

3. Twin experiment 1

In the course of data assimilation by using the adjoint variational method, we must calculate the gradient of cost function with respect to control variables. The cost function declines in the inverse direction of its gradient, and the gradient is used to adjust the control variables. The adjustment is: $x_{k+1} = x_k + \alpha_k \cdot d_k$, in which k is the assimilation step, d_k is the direction (inverse direction of gradient of cost function), and α_k is step-length that is the amount to modify the control variables.

The purpose of experiments in this section is to improve assimilation efficiency by designing a better step-length that is used to modify the parameters. The spatial variation of Vm is set to type 1, and the other four parameters remain unchanged. Run the model for five days and the simulated phytoplankton in the surface layer are recorded as model generated ‘observations’. Hereafter, these ‘observations’ are assimilated into the model to estimate the given spatial variation of Vm . We adjust Vm in according to this form: $Vm_{k+1} = Vm_k + \alpha_k \cdot d_k$, where $d_k = -Vm \cdot 5\%/86400 \cdot G_k / |G_k|$, G_k is the gradient of cost function

with respect to V_m . There are 42×42 independent grids (1142 wet grids) distributing uniformly over each $3^\circ \times 3^\circ$ study area.

3.1. The first strategy: previous method

The first strategy used to defined the value of α_k to adjust the parameter is similar to the work of Fan and Lv [14], that is $\alpha_k = 1.01 - 0.01k$, where k is assimilation step. We analyze the experimental results with the influence radius ranging from 5° to 12° to explore the interference brought by influence radius. When the influence radius is 9° , assimilation results is the most optimal: ME achieves the minimum $0.0038 \text{ mmol-N m}^{-1}$, AAE of V_m drops to 0.0032 day^{-1} from 0.157 day^{-1} and RCF is 0.027 after 28 steps (see Table 2). We can see RCF dose not decrease with assimilation steps obviously and fluctuates after 6 steps (see Fig. 3). We attribute this to the improper amount of the modification of parameter because the step-length is very important, and affects the assimilation efficiency and simulative accuracy of simulation. So we design better strategies of optimizing the step-length to improve assimilation efficiency.

Table 2. The results of the first strategy

Influence radius ($^\circ$)	ME (mmol-N m^{-1})	RCF	V_m AAE (day^{-1})
5	0.0048	0.154	0.045
6	0.0039	0.046	0.032
7	0.0042	0.040	0.034
8	0.0042	0.034	0.033
9	0.0038	0.027	0.033
10	0.0039	0.030	0.033
11	0.0039	0.029	0.035

3.2. The second strategy

From Table 2 we can see that the optimal influence radius is 9° when there are 42×42 independent grids in the study area, so 8° and 9° are chosen as influence radius in this section, which reduces times of experiments and provides reference value for real experiments in future. We find the RCF fluctuates regularly after 5 steps when $\alpha_k = 1$, ($k=1, 2, 3, \dots, 28$), and five groups of experiments are carried out to compare the simulated results with different α_k (see Table 3).

The ME, RCF and AAE of V_m all get minimum value in group 3 where $\alpha_k = (0.7)^{k-5}$, $k > 5$, whether the influence radius is 9° or 8° . The RCF is 0.0008 that is 2 orders of magnitude smaller and the ME also reduces to $0.0005 \text{ mmol-N m}^{-3}$ that is 1 order of magnitude smaller than the result of the first strategy mentioned above. The AAE of V_m is 0.021 after assimilation, indicating that the given type of spatially varying V_m is reproduced better.

Table 3. Results of the second strategy.

Group of experiment	α_k		influence radius is 8°			influence radius is 9°		
	$k < 6$	$5 < k < 29$	ME (mmol·N m ⁻³)	RCF	Vm AAE (day ⁻¹)	ME (mmol·N m ⁻³)	RCF	Vm AAE (day ⁻¹)
1	1	$(0.5)^{k-5}$	0.0008	0.002	0.022	0.0007	0.002	0.022
2	1	$(0.6)^{k-5}$	0.0006	0.001	0.022	0.0006	0.001	0.021
3	1	$(0.7)^{k-5}$	0.0005	0.0008	0.021	0.0005	0.0009	0.021
4	1	$(0.8)^{k-5}$	0.0007	0.002	0.023	0.0008	0.002	0.023
5	1	$(0.9)^{k-5}$	0.0021	0.009	0.029	0.0021	0.009	0.028

3.3. The third strategy

8° is chosen as the optimal influence radius to compare results of experiments when there are 42×42 independent grids, because it has less impact on the result obtained with the influence radius that is 8° or 9° , which is demonstrated in section 3.2. After discussion we design the third strategy in which step-length gradually decreases with different speed in different scope of step (see as follows).

$$\alpha_k = 1 - 0.1(k-1), k=1, 2, 3, \dots, 10;$$

$$\alpha_k = 0.1 - 0.01(k-10), k=11, 12, \dots, 19;$$

$$\alpha_k = 0.01 - 0.001(k-19), k=20, 21, \dots, 28.$$

After 28 steps, the RCF, EM and AAE of Vm are reduced to 0.0004, 0.0002 mmol·N m⁻¹ and 0.020 day⁻¹ respectively.

The RCF, ME and AAE of Vm get minimum value at same time under the condition of optimal influence radius (8°) in all the three strategies above that are shown in Fig. 3. The left one is the values of step-length in different strategies while the right one is the corresponding RCF values in logarithmic coordinate system. It can be obviously seen that after 5 steps there is fluctuation in the results of the first strategy and that the RCF decreases slowly and is reduced to 0.03 until the 28th step. While there is no fluctuation in the result of the second strategy and more importantly it is of higher efficiency that the RCF drops to a degree of 0.0008 in the 6th step while dozens or hundreds steps may be required in the first strategy. But it takes less effect after 16 steps. The third strategy is better not only in efficiency but also in precision, because the values of RCF and ME decrease by half compared with the results of the second strategy. The reproduced spatial variation of Vm by the first strategy is mainly consistent with the given type of Vm , but not smooth as the results of other two strategies which are more consistent with the given type except for the region at high latitude based on the comparison in Fig. 4 Fig. 5 shows the Vm AAE between reproduced values and given values of every grid point in the whole study area by which it can be further demonstrated that the Vm AAE of the second strategy is relatively bigger in part area of middle latitude than the third one. So with regard to modifying the parameters, we summarize that: firstly, the step-length should decrease gradually; secondly, fluctuation of the results and inefficiency may appear owing to the step-length decreasing with a constant speed; furthermore, the step-length may tend to zero after several steps which has little or no effect on modifying the parameters if it decreases with a speed of decimal power exponent (e.g. $(0.7)^{k-5}$ in this study); finally, step-length gradually decreasing with different speed in different scope of step is relatively optimal in terms of computational efficiency and precision.

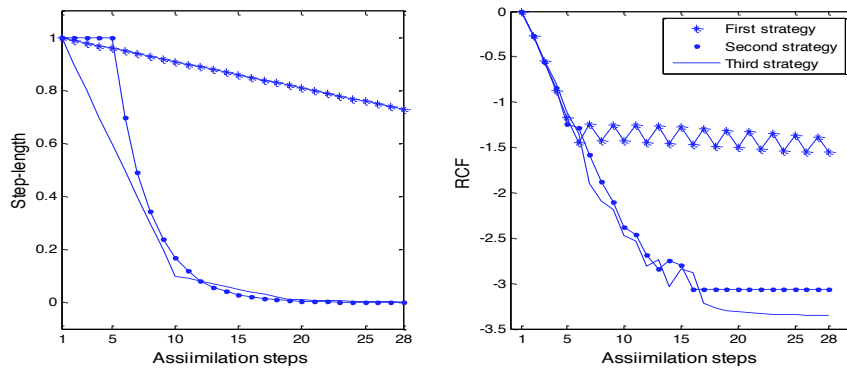


Fig. 3. The comparison of all the three strategies. The step-length are shown on the left, while the figure shown on the right is corresponding RCF.

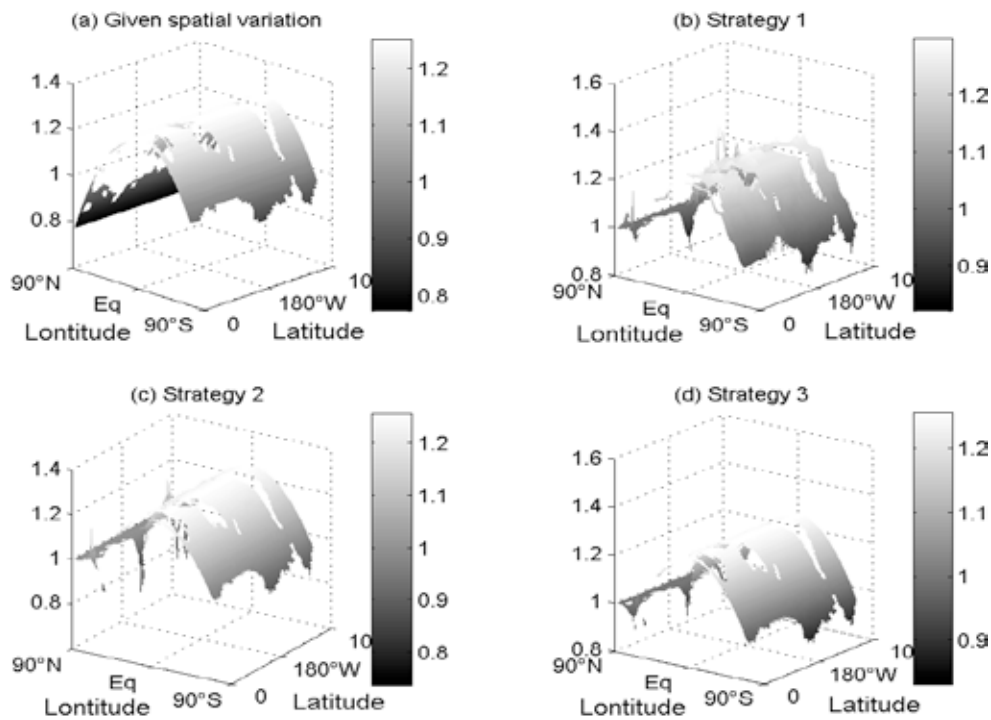


Fig. 4. Inversion results of the three strategies. Fig. 4(a) shows the variation of spatial variation 1; Fig. 4(b) ~ Fig. 4(d) are the inversion results of the three methods respectively.

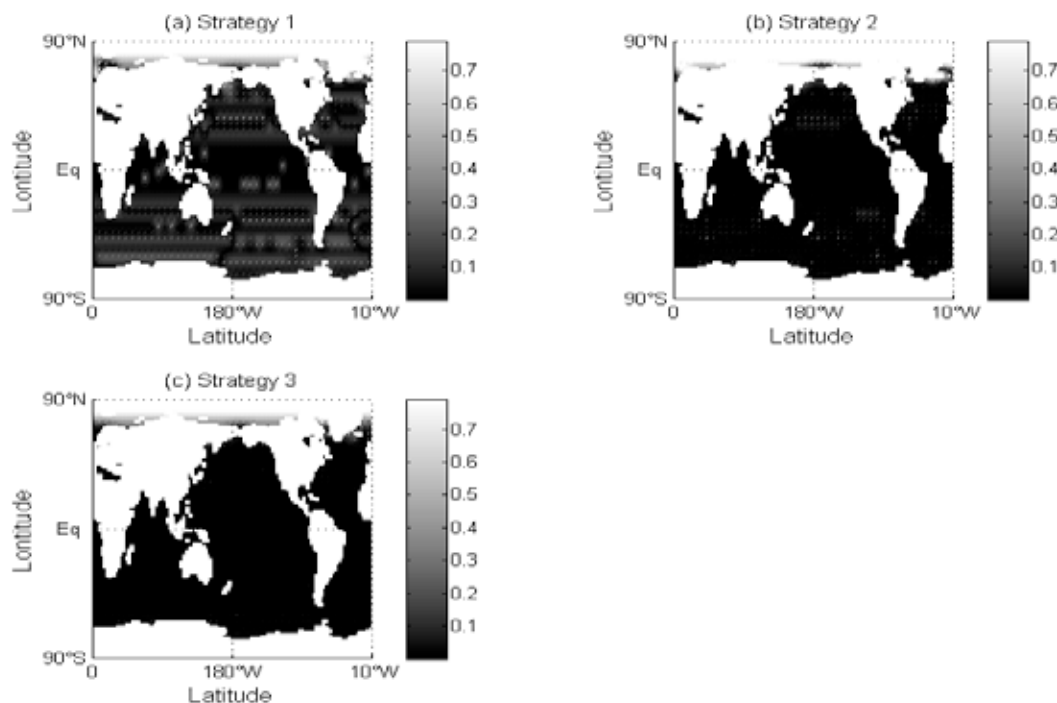


Fig. 5. The misfits between the inverted and given parameter.

4. Twin experiment 2

The values of RCF in logarithmic coordinate system are shown in Fig. 6 for the experiments of five schemes. We can see obviously that RCF all decreases as the influence radius increases with a interval of 1° at first, and reaches the minimum when the influence radius is the optimal value, then RCF begins to increase as the influence radius continue to rise. The optimal influence radius is different for each scheme (see Table 4). It is demonstrated that parameters in marine ecosystem has a local feature. There may be no efficient grids for interpolation in the scope of the given influence radius or some contributive grid points are not involved in interpolation since the radius is too small. On the other hand, if the influence radius is too large, there will be more errors because there are more grid points involved in interpolation including some grid points that have no influence. So it may reduce the simulation accuracy either the influence radius is too small or too large. The inverted results are shown in Table 4 in the case using the optimal influence radius, which is ranked in the order of 'A', 'B', 'C', 'D', 'E' successively. We can get the conclusion that the more independent grids we use, the better the assimilation results are which is in accordance with the work of Fan and Lv [14].

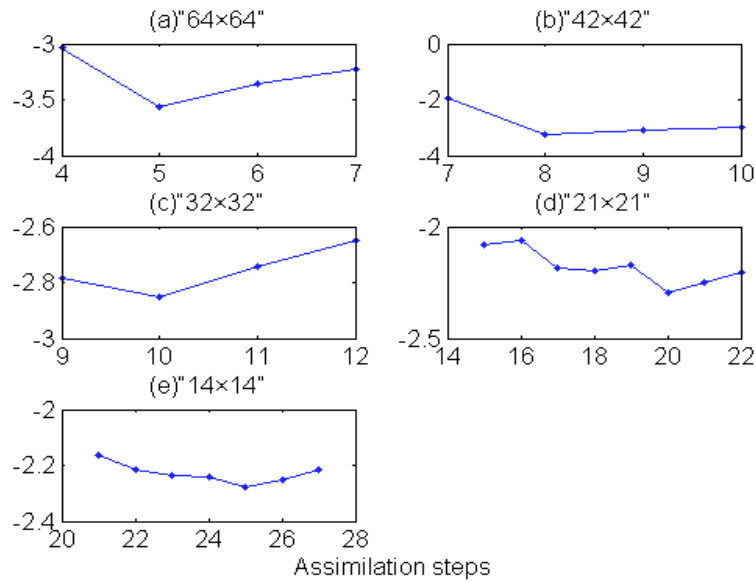


Fig. 6. Values of RCF in different schemes of independent grids.

Table 4. Results from different schemes of independent grids.

Schemes	Wet grids	Optimal radius(°)	RCF of V_m	ME ($\text{mmol} \cdot \text{N} \cdot \text{m}^{-3}$)
A	2606	5	0.0002	0.0001
B	1142	8	0.0004	0.0002
C	642	10	0.001	0.0005
D	288	20	0.004	0.0009
E	138	24	0.004	0.0011

5. Twin experiment 3: Inversion of spatially variable V_m , G_m , D_p , D_z , e

We get the optimal strategy of modifying the step-length and 'A' scheme of independent grids including the corresponding influence radius by reproducing one type of spatial varying V_m in the two sections above. Based on these conclusions, the two spatial variations are given to one of the five parameters in Table 1, and the other four parameters remain unchanged. Since each parameter has two given types of spatial variations, there are ten inversions in all.

Table 5 shows the results of the ten inversions. For each parameter, the two given types of parameter variations can be estimated successfully, and the mean relative errors of the estimated parameters are less than 3%. The RCF can drop to magnitude of 10^{-6} at most and the ME of phytoplankton in the surface

layer is basically two orders of magnitude smaller than before indicating that spatially varying parameters can be effectively estimated by the adjoint variational method and the improvements in above study are applicative. Fig. 7 and Fig. 8 show the reproduced parameters of the given type 1 and 2, respectively. Several estimated parameters have bigger errors in some subpolar regions in the Northern Hemisphere. This is because the level of phytoplankton in these areas in the initial fields is very low. The twin experiments are only a model run of five-day long from initialization, so the simulated level of phytoplankton remains low. Therefore, assimilating such ‘observations’ will give less constraint to the estimation of the parameters.

Table 5. Inversion results of five parameters

(a) Type 1

Estimated parameter	RCF	ME (mmol·N m ⁻³)		RAE	
		Before assimilation	After assimilation	Before assimilation	After assimilation
<i>V_m</i>	0.0002	0.030	0.0001	0.139	0.024
<i>D_p</i>	0.14	0.020	0.0005	0.139	0.003
<i>G_m</i>	0.000005	0.018	0.00002	0.139	0.025
<i>e</i>	0.0005	0.002	0.00001	0.139	0.025
<i>D_z</i>	0.000005	0.001	0.000002	0.139	0.027

(b) Type 2

Estimated parameter	RCF	ME (mmol·N m ⁻³)		RAE	
		Before assimilation	After assimilation	Before assimilation	After assimilation
<i>V_m</i>	0.0003	0.027	0.0002	0.189	0.017
<i>D_p</i>	0.0006	0.021	0.00017	0.189	0.002
<i>G_m</i>	0.000004	0.035	0.00004	0.189	0.021
<i>e</i>	0.0005	0.002	0.00001	0.189	0.019
<i>D_z</i>	0.56	0.001	0.00007	0.189	0.023

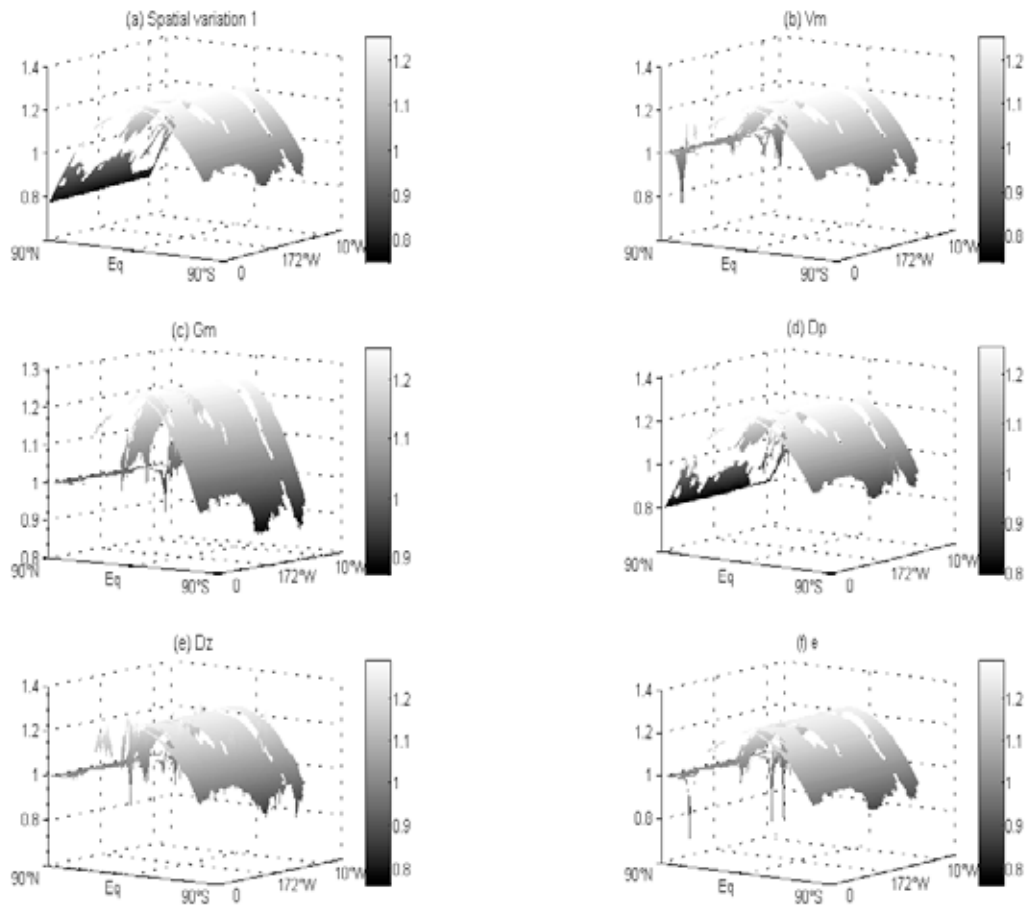


Fig. 7. Inversion results of spatial variation 1. Fig. 7(a) shows the variation of spatial variation 1; Fig. 7(b) ~ Fig. 7(f) are the inversion results of the five parameters.

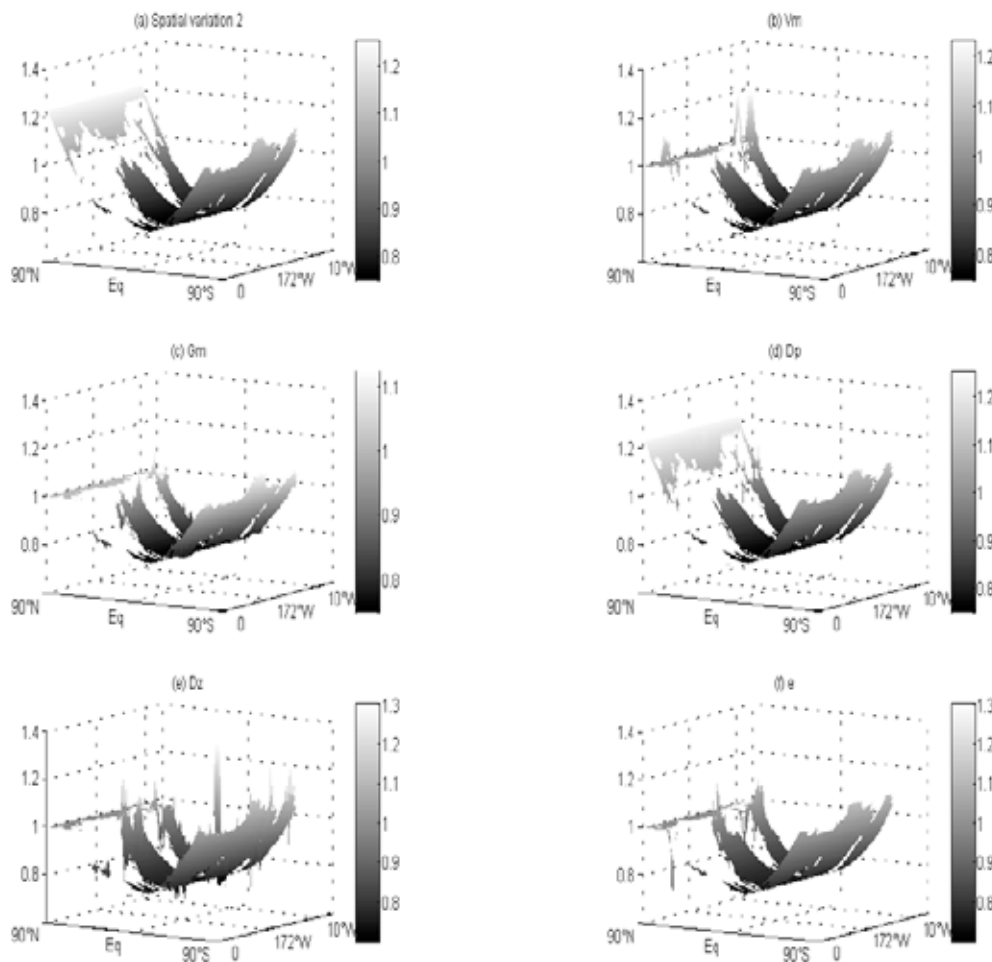


Fig. 8. Inversion results of spatial variation 2. Fig. 8(a) shows the variation of spatial variation 2; Fig. 8(b) ~ Fig. 8(f) are the inversion results of the five parameters.

6. Conclusion

The adjoint variational method is applied to numerical simulation of marine ecosystem dynamics based on the spatial parameterizations in this study, since a set of constant parameters in marine ecosystem modeling and parameter estimation on global scales is questionable. On the basis of previous studies, we make some improvements to the strategy used for adjusting the parameters and conduct discussion in detail.

The spatially varying V_m (maximum uptake rate of nutrient by phytoplankton) is reproduced alone by assimilating chlorophyll-a data in the twin experiment 1. New strategies are designed to modify the step-length and are used to adjust the parameters preferably and the assimilation efficiency is improved. When the assimilation steps are equal, compared with result of strategy in previous work, the RCF is 0.00058 that is 2 orders of magnitude smaller than 0.027 (previous result), and the ME also reduces to 0.0004 mmol-N m^{-3} . The misfit of V_m between reproduced values and given values decreases obviously.

Based on the optimal strategy for modifying the parameter, the distribution schemes of spatial parameterization and how the influence radius affects the results are discussed. The optimal influence radius corresponding to each distribution scheme is obtained. We draw the same conclusion as Fan and Lv [14] that the more independent grids we use, the better the assimilation results are. On the basis of the above work, when the five key parameters V_m , G_m , D_p , D_z , e which mainly influence ecological mechanisms are estimated separately, the two given types of their spatial variations could be reproduced, and the RAE is less than 3% for every parameter.

It is demonstrated that the adjoint assimilation method based on spatial parameterizations is an effective tool to estimate parameters in marine ecosystem. The simulation precision and efficiency are improved by utilizing the improved strategy for modifying the step-length and the distribution schemes of independent grids to achieve spatial parameterization. The improvements achieved in this study provide instructive significance and a big boost for research of numerical simulation in marine ecosystem dynamics in future.

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